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Search Results -

Term	Documents
US-6149837-$	0
US-6149837-A.DWPI,EPAB,JPAB,USPT.	2
US-6149837-$.DID..USPT,JPAB,EPAB,DWPI,TDBD.	2
(US-6149837-$.DID.).USPT,JPAB,EPAB,DWPI,TDBD.	2

Database: US Patents Full-Text Database; US Pre-Grant Publication Full-Text Database; JPO Abstracts Database; EPO Abstracts Database; Derwent World Patents Index; IBM Technical Disclosure Bulletins

Search: L5

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Search History

DATE: Thursday, September 19, 2002 Printable Copy Create Case

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DB=USPT,JPAB,EPAB,DWPI,TDBD; PLUR=YES; OP=ADJ			
L5	us-6149837-$.did.	2	L5
L4	us-6149387-$.did. or us-6030546-$.did.	4	L4
L3	us-6294231-$.did.	2	L3
L2	jp-2000273205-$.did.	2	L2
L1	de-4105742-$.did.	2	L1

END OF SEARCH HISTORY

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L1: Entry 2 of 2 File: DWPI Aug 9, 2001

DERWENT-ACC-NO: 1992-293267
DERWENT-WEEK: 200145

TITLE: 2,6-Di:fluoro-tolan derivs. - useful as components of liq. crystal media for electro=optical displays

INVENTOR: PLACH, H; REIFFENRATH, V

PRIORITY-DATA: 1991DE-4105742 (February 23, 1991), 1991DE-4143657 (February 23, 1991)

PATENT-FAMILY:

PUB-NO	PUB-DATE	LANGUAGE	PAGES	MAIN-IPC
DE 4105742 C2	August 9, 2001		000	C07C043/225
DE 4105742 A	August 27, 1992		019	C07C043/225
DE 4143657 A1	October 5, 2000		000	C09K019/18

INT-CL (IPC): C07C 25/24; C07C 43/225; C07C 69/00; C07C 255/00; C07C 323/00; C07D 213/24; C07D 239/24; C07D 319/06; C09K 19/06; C09K 19/18; C09K 19/30; C09K 19/34; G02F 1/13; G02F 1/137; G09F 9/35

ABSTRACTED-PUB-NO: DE 4105742A
BASIC-ABSTRACT:

2,6-Difluorotolans of formula (I) are claimed. R1, R2= 1-18C alk(en)yl, opt. with 1 or 2 non-adjacent CH2 gps. replaced by O, S, COO or OCO; one of these gps. can also = F, Cl, CN, CF3, OCF3 or OCF2H; A1, A2= 1,4-cyclohexylene, 1,4-phenylene, 2- or 3-fluoro-1,4-phenylene, 2,3-difluoro- 1,4-phenylene, 2,6- or 3,5-difluorophenylene, dioxan-2,5-diyl, pyridine-2,5-diyl or pyrimidine-2,5-diyl; Z1, Z2= -CH2CH2-, -(CH2)4-, -CH2O-, -OCH2-, -CC- or a single bond; m, p = 0, 1 or 2; o= 0, 1 or 2.

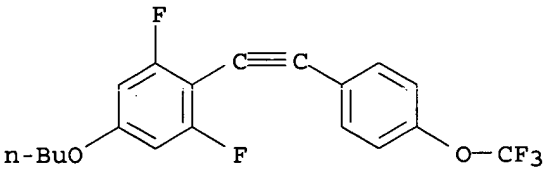
USE/ADVANTAGE - (I) are useful as components of liq. crystal (LC) media for electro-optical displays. Also claimed are LC media with at least 2 components, at least one of which contains a 2,6-difluorotolan gp. as in (I), pref. a cpd. of formula (I), and electro-optical displays contg. such LC media. The incorporation of (I) gives stable LC media with relatively high optical anisotropy and pronounced positive dielectric anisotropy, useful esp. in TNC-based display elements; cpds. (I) have high chemical, thermal and light stability, and form LC mesophases in the relevant temp. range.

-

RN 144891-35-0 REGISTRY
CN Benzene, 5-butoxy-1,3-difluoro-2-[[4-(trifluoromethoxy)phenyl]ethynyl]-
(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H15 F5 O2
SR CA
LC STN Files: CA, CAPLUS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2



Calculated Properties (CALC)

CODE	PROPERTY	VALUE	CONDITION	NOTE
HD	H donors	0		(1) ACD
HAC	H acceptors	2		(1) ACD
MW	Molecular Weight	370.31		(1) ACD
LOGP	logP	7.616+/-0.782		(1) ACD
FRB	Freely Rotatable Bonds	6		(1) ACD
LOGD	logD	7.62	pH 1	(1) ACD
LOGD	logD	7.62	pH 4	(1) ACD
LOGD	logD	7.62	pH 7	(1) ACD
LOGD	logD	7.62	pH 8	(1) ACD
LOGD	logD	7.62	pH 10	(1) ACD
SLB.MOL	Molar Solubility	<0.01 mol/L	pH 1	(1) ACD
SLB.MOL	Molar Solubility	<0.01 mol/L	pH 4	(1) ACD
SLB.MOL	Molar Solubility	<0.01 mol/L	pH 7	(1) ACD
SLB.MOL	Molar Solubility	<0.01 mol/L	pH 8	(1) ACD
SLB.MOL	Molar Solubility	<0.01 mol/L	pH 10	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2002 ACD)

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

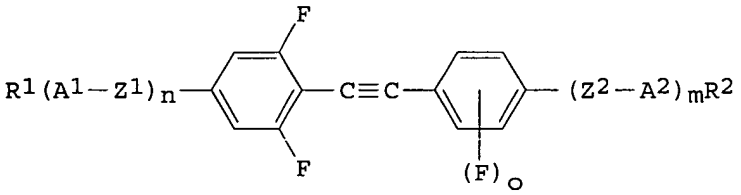
REFERENCE 1

AN 118:59406 CA
TI 2,6 difluorotolane
IN Reiffenrath, Volker; Plach, Herbert
PA Merck Patent G.m.b.H., Germany
SO Ger. Offen., 19 pp.
CODEN: GWXXBX

DT Patent
LA German
IC ICM C07C043-225
ICS C07C025-24; C09K019-06; G09F009-35; G02F001-13; C07D319-06; C07D213-24; C07D239-24
ICA C09K019-18; C09K019-30; C09K019-34; C09K019-20; C09K019-58; C07D521-00; C07D401-10; C07D401-12; C07D405-10; C07D405-12
CC 25-3 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4105742	A1	19920827	DE 1991-4105742	19910223
DE 4105742	C2	20010809		

GI



I

AB A process was developed for the prepn. of 2,6-difluorotolane of formula I [R1, R2 = alkyl or alkenyl, A1, A2 = 1,4-cyclohexylene, -phenylene, 2- or 3-fluoro-1,4-phenylene, Z1, Z2 = CH2CH2, -CH2O-, (CH2)4, m, n, o = 1-2] as a component of liq. crystal medium having electrooptical properties. E.g., the treatment of 3,5-difluoropentylbenzene (0.129 mol) with 114 mL THF and BuLi followed by 4-ethoxyacetophenone (0.129 mol) gave a product mixt. which was treated with p-toluenesulfonic acid (4 g) in toluene. Subsequent reaction of product mixt. with .09 mL bromine in EtOAc and with 12.6 mL Et3N and then reaction with LDA in THF gave final product 4-pentyl-2,6-difluoro-4'-ethoxytolane.

ST fluorotolane electrooptical property; acetylene difluoro diphenyl; palladium catalyst coupling fluorophenylacetylene iodobenzene

IT Coupling reaction
(of difluorophenylacetylene with trifluoromethoxyiodobenzene and analogs, difluorotolanes from)

IT Coupling reaction catalysts
(palladium compds., for the coupling of difluorophenylacetylene with trifluoromethoxyiodobenzene and analogs, difluorotolanes from)

IT 144890-97-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(3)

IT 14221-01-3
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for the coupling of difluoroiodobenzene derivs. with fluorophenylacetylene)

IT 13965-03-2
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for the coupling of difluorophenylacetylene deriv. with trifluoromethoxyiodobenzene)

IT 628-17-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reaction of, with difluorobromobenzene)

IT 461-96-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reaction of, with iodopentane)

IT 103962-05-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(coupling reaction of, with difluorophenylacetylene deriv.)

IT 766-98-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(coupling reaction of, with ethoxydifluoroiodobenzene)
IT 144911-50-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(coupling reaction of, with trifluoromethoxyiodobenzene)
IT 144891-25-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(iodination of)
IT 144891-24-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and coupling of, with fluorophenylacetylene)
IT 40817-08-1P 41122-70-7P 52709-83-8P 58743-75-2P 58743-76-3P
61203-99-4P 61204-01-1P 79832-84-1P 80944-44-1P 80955-71-1P
81936-32-5P 85600-56-2P 134143-76-3P 144890-96-0P 144890-98-2P
144890-99-3P 144891-00-9P 144891-01-0P 144891-02-1P 144891-03-2P
144891-04-3P 144891-05-4P 144891-06-5P 144891-07-6P 144891-08-7P
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144891-14-5P 144891-15-6P 144891-16-7P 144891-17-8P 144891-18-9P
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144891-46-3P 144891-47-4P 144891-48-5P 144891-49-6P 144891-50-9P
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144891-61-2P 144891-62-3P 144891-63-4P 144891-64-5P 144891-65-6P
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RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT 144911-67-1P 144911-68-2P 144911-69-3P 144911-70-6P 144911-71-7P

144911-72-8P 144911-73-9P 144911-74-0P 144922-37-2P 144922-38-3P
144922-39-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT 1676-63-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with difluoro(pentyl)benzene)

IT 121219-25-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with ethoxyacetophenone)